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Applied Mathematics
Biometrics
and Process Control

EPAS n.v.

Adequate Complexity for Biofilm Systems Modelling

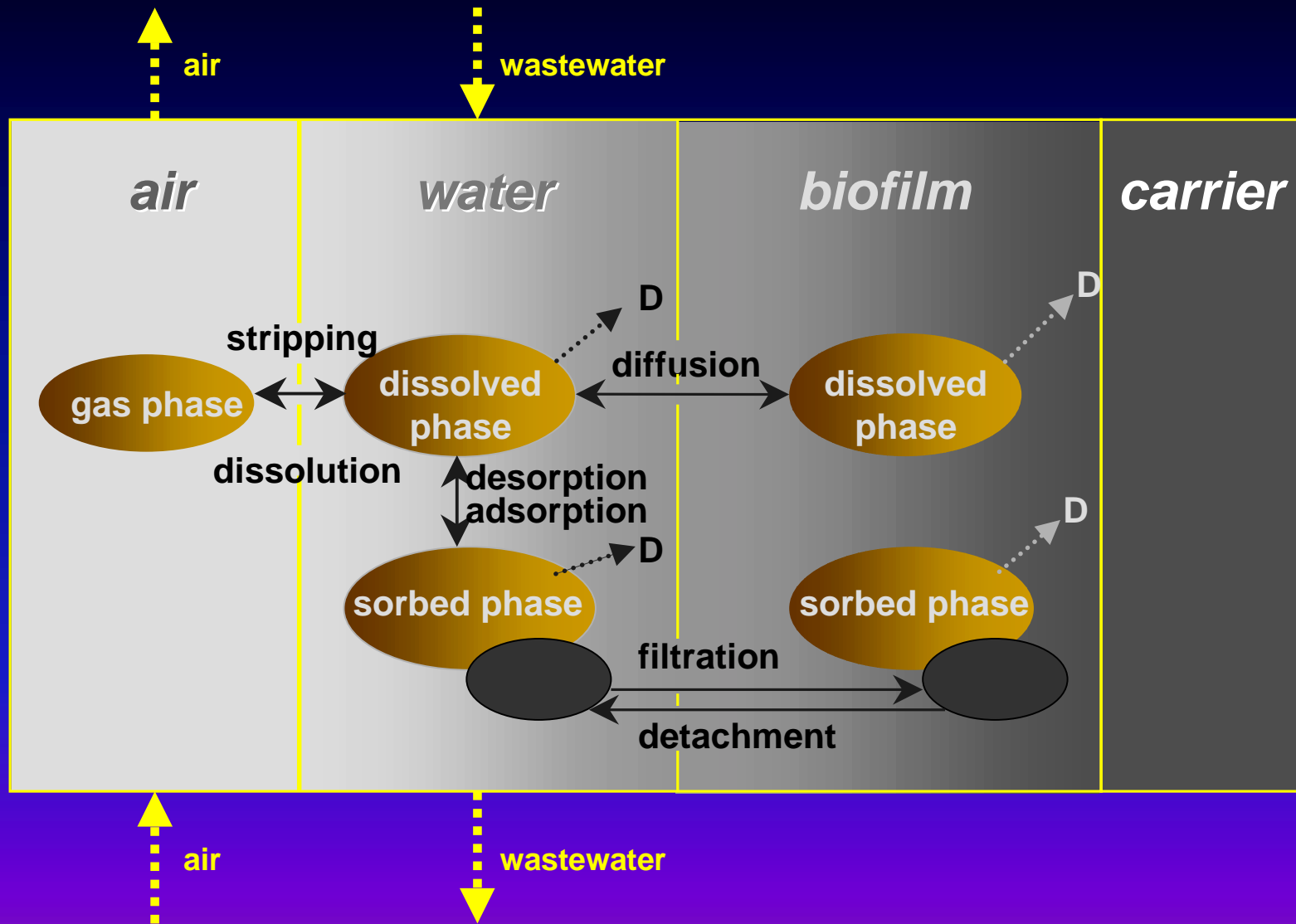
Henk Vanhooren and Peter A. Vanrolleghem

Biofilms: Modelling and Analysis of Structure and Activity
Wageningen, November 17 2000

Cases Studies with Biofilm Models

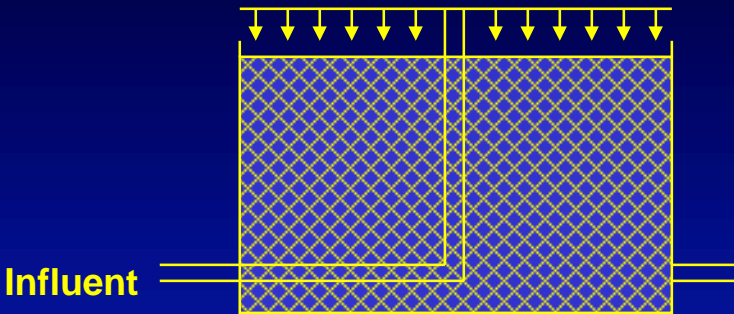
- Biofilm Reactors
- Why Model Biofilm Systems
- Biofilm Models Available
- Practicle Modelling Needs and Difficulties
- Case Study 1 and 2
 - The Aim
 - Model Building, Extension and Implementation
 - Results
- Conclusions

Biofilm Reactors

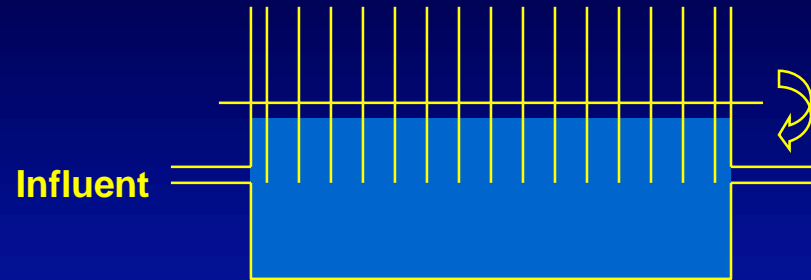


Some Biofilm Reactor Types

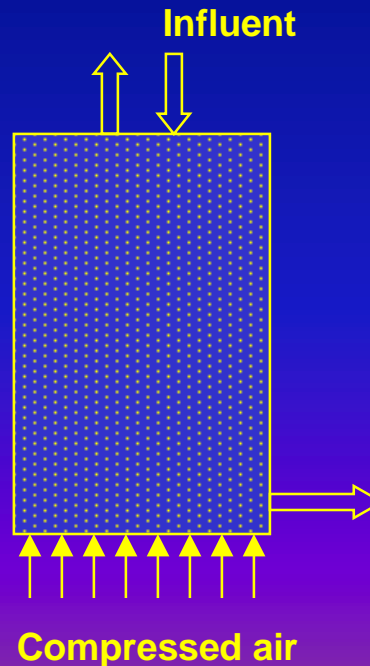
Trickling filter



Rotating biological contactor



Aerated submerged filter

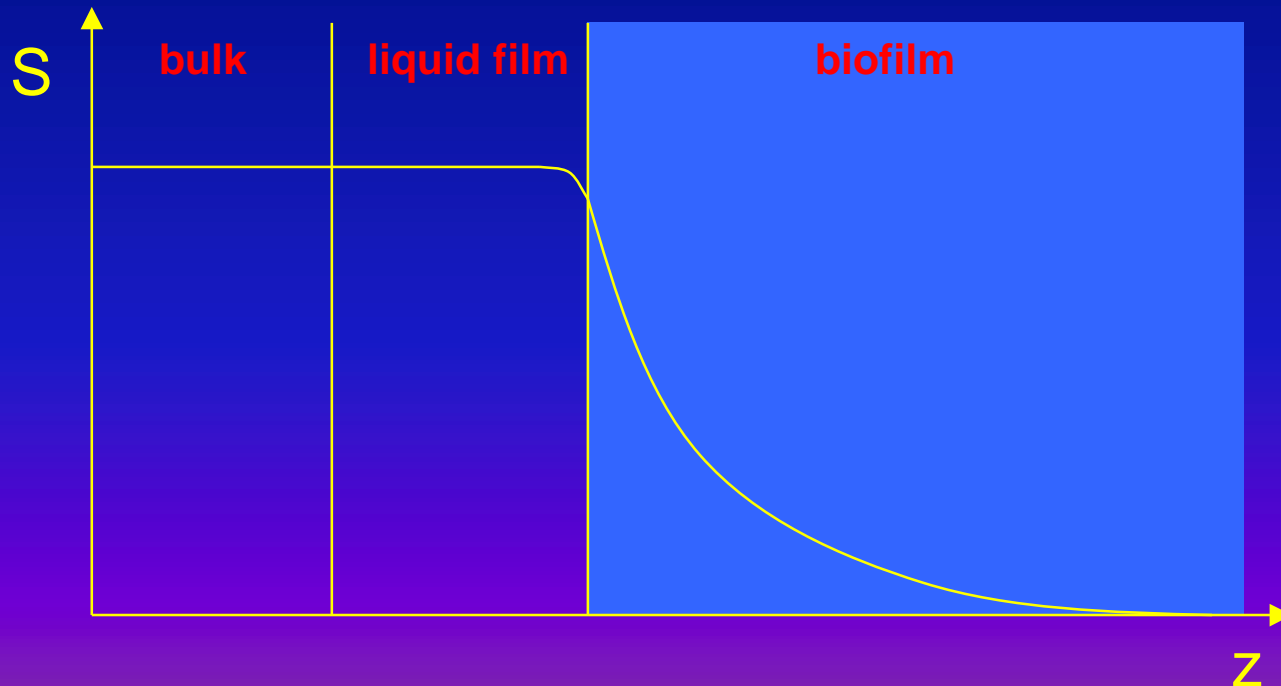


Why Model Biofilm Systems

- Models are tools to develop understanding of complex interactions in biological systems
- Model applications
 - Qualitatively: improve general system understanding
 - Quantitatively: describe dynamic system responses
- Very few models used by practitioners (WWT)
 - Task: clarify when mathematical models can be helpful

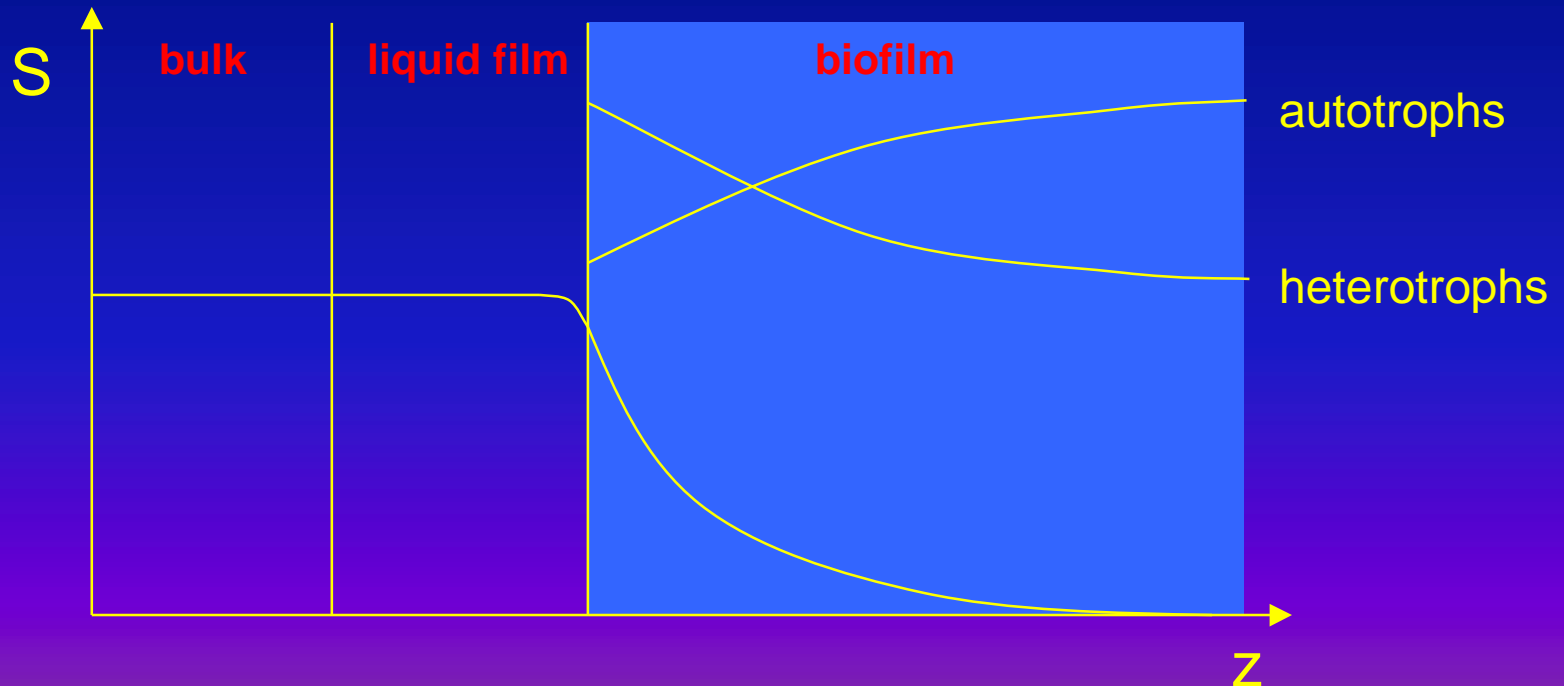
Biofilm Models Available (1)

- 1D models focussing on substrate gradients (uniform biomass distribution)
 - Describe mass transport limitations to the biofilm
 - Analytical solutions or ODE-models: relatively simple



Biofilm Models Available (2)

- 1D models focussing on biomass distribution
 - Describe competition of different species
 - PDE-models



Biofilm Models Available (3)

- Multi-dimensional models
 - Heterogeneous biomass and substrate distribution in 2 or 3 dimensions
 - High performance computing necessary

Practical Modelling Needs

- Describe plant dynamics
 - Response to influent variations
 - Off-line optimisation via scenario-analysis
 - On-line control and optimisation (real-time simulation)
- Troubleshoot
 - Give answers to practical questions on how to operate the plant
- Reactor design
 - Evaluate data from pilot plant
 - Predict full-scale operation

Difficulties of Practical Application (1)

High model complexity

- Considerable detail at the micro-scale
 - Influence of micro-scale on macro-scale reactor performance?
 - Too detailed for practical (on-line) applications
- Still, quite some important processes are poorly described:
 - Attachment and detachment, clogging and backwashing, influence of higher organisms, flow distribution, ...
- A lot of parameters need to be calibrated. Most of them can not be measured directly

Difficulties of Practical Application (2)

Low model complexity

- Not able to describe all the dynamics of the system because of simplifications
- Lower amount of parameters: calibration easier

Adequate complexity: good balance between pro's and con's of different models

Case Study: The Aim

is to use
BIOFILM MODELS

to

improve the UNDERSTANDING of the
COMPLETE BIOFILM BASED PROCESS UNIT

and

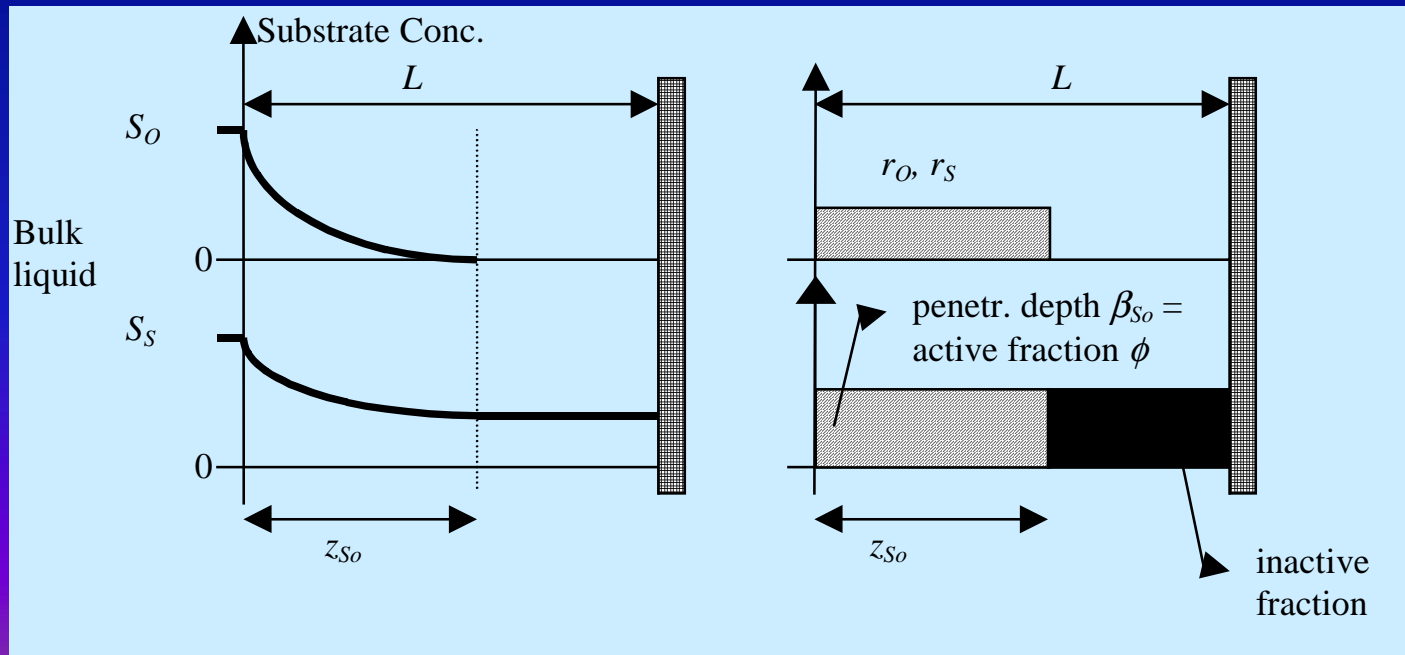
to OPTIMISE the process where possible

Model Building: a complexity compromise

MODEL : Rauch, Vanhooren & Vanrolleghem (1999)

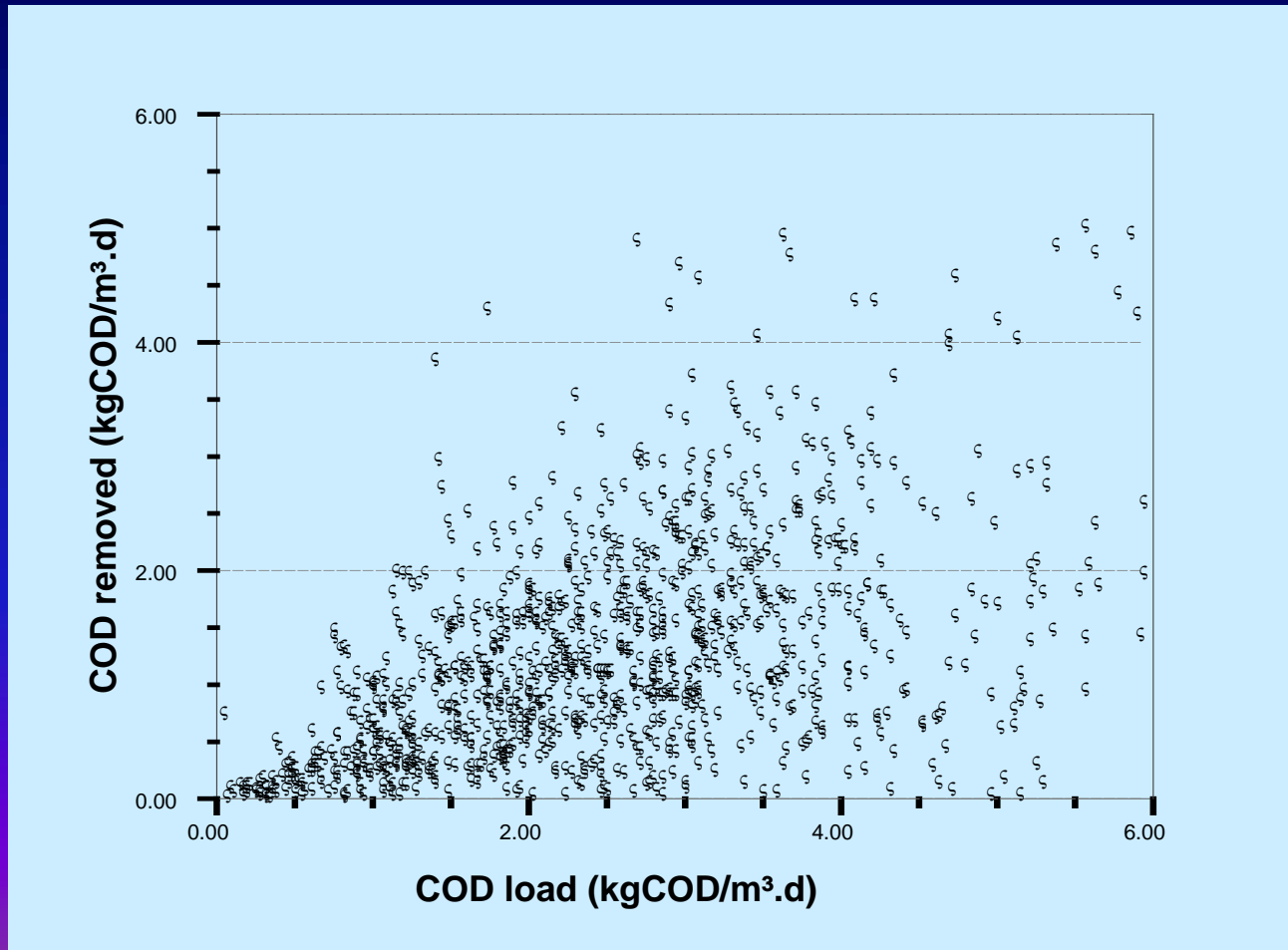
Model solved by a two step procedure

- (1) the active fraction of the biomass within the biofilm is computed
- (2) all conversions within the biofilm are calculated using only the active fraction of the biomass in the biofilm



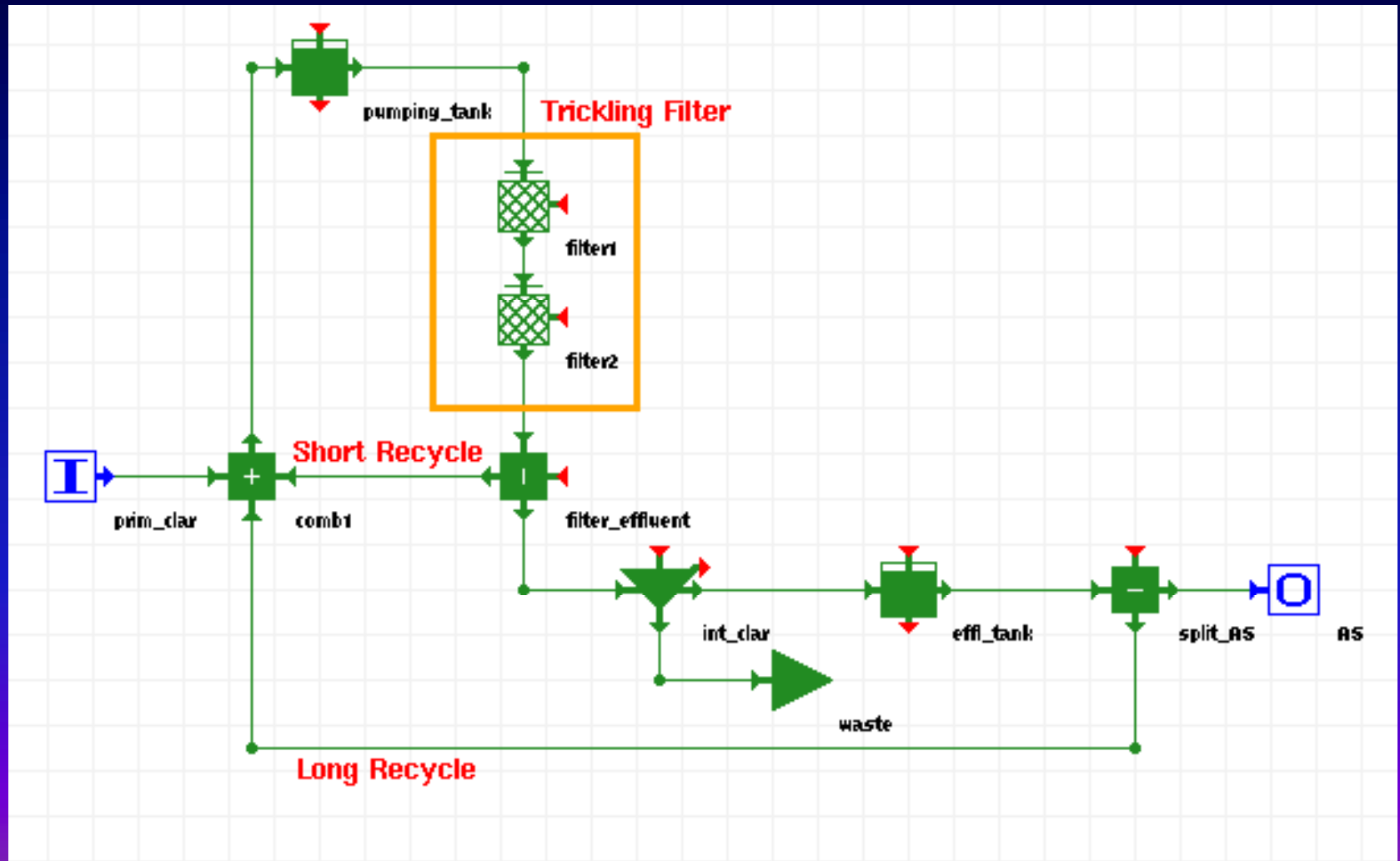
Case Study 1 (1)

- Trickling filter treating mainly domestic sewage wastewater
- COD load vs. COD removal:



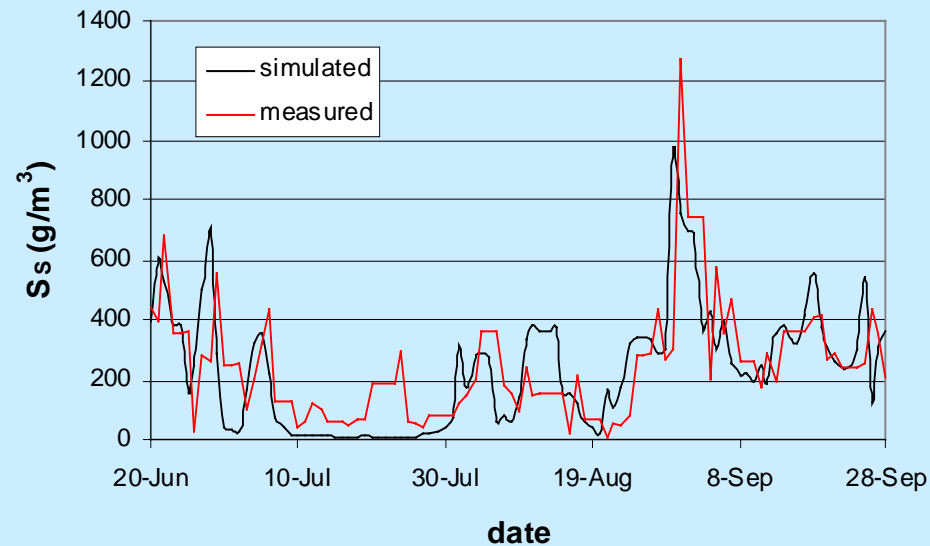
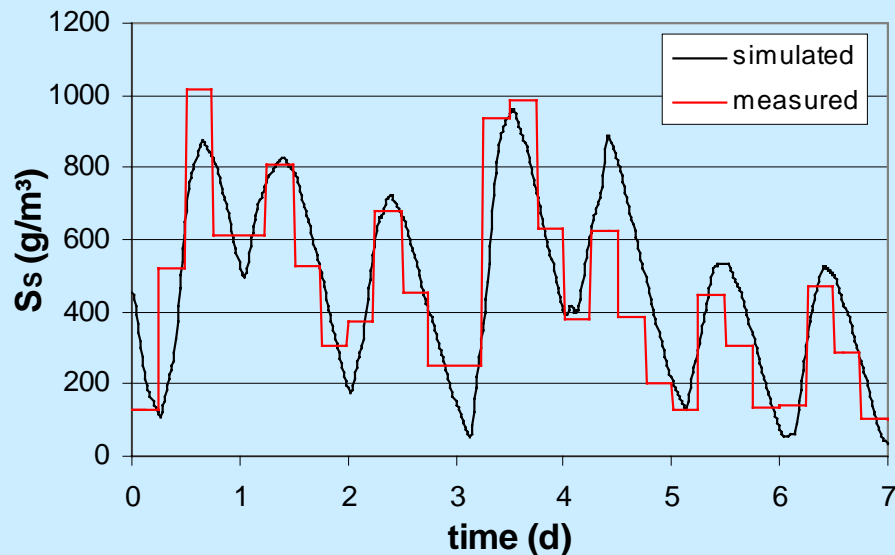
Case Study 1 (2)

Model Implementation (WEST[®])



Case Study 1 (3)

- Calibration and validation, only off-line measurements
- Further model simplification: only carbon removal



- Maximum COD removal modelled : 2 kg COD / m³.d
<-> measured COD removal ??
- Be careful using point measurements.

Case Study 2 (1)

- Filter treating highly loaded industrial wastewater
- Load : 15000 kg COD/d
- Reactor Volume : 3160 m³
- Average Flow Rate : 110 m³/h
- Air Flow Rate
 - high flow : 17300 m³/h
 - low flow : 10900 m³/h

Case Study 2 (2)

ON-LINE Measurement Techniques

respirometry

- RODTOX biosensor (Kelma bvba, Niel, Belgium)
- Load and toxicity monitoring
- Estimation of readily biodegradable COD

off-gas analysis: O₂ and CO₂

- Measurement is indication for complete reactor performance
- Clean and robust : no fouling, no chemicals, ...
- Can be used to study
 - Oxygen and carbon mass balances.
 - Changes in load and process behaviour.

Case Study 2 (3)

Model Extension

extension for I/C production and transport

$CTR^{measured}$

↑

$CO_2^{(gas)}$

⇌

$CPR^{reality}$

↓

$CO_2^{(aq)}$

⇌

H_2CO_3

⇌

$HCO_3^- + H^+$

⇌

$CO_3^{2-} + 2H^+$

kinetic modelling of CO_2 / HCO_3^- equilibrium
necessary : hydration of $CO_{2(aq)}$ is slow !!

Case Study 2 (4)

Model Calibration

1. sludge balance : attachment / detachment

SS and NH_4^+

2. effluent concentrations : growth / decay / yield

basic question : oxygen or substrate limited system ??

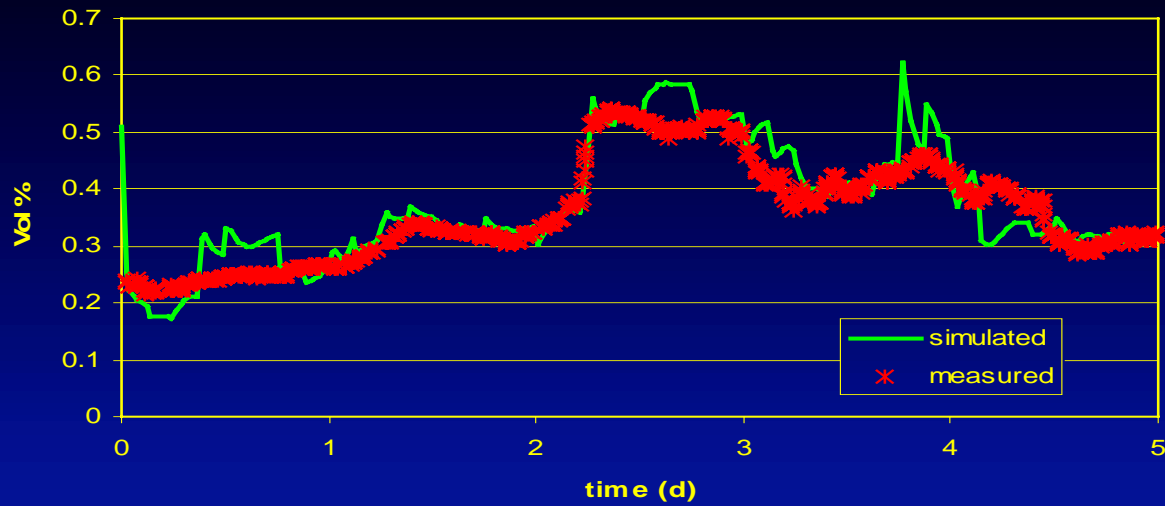
model predicts substrate limitation in $\pm 50\%$ of time

3. off-gas concentration : $K_L a$ for O_2 and CO_2

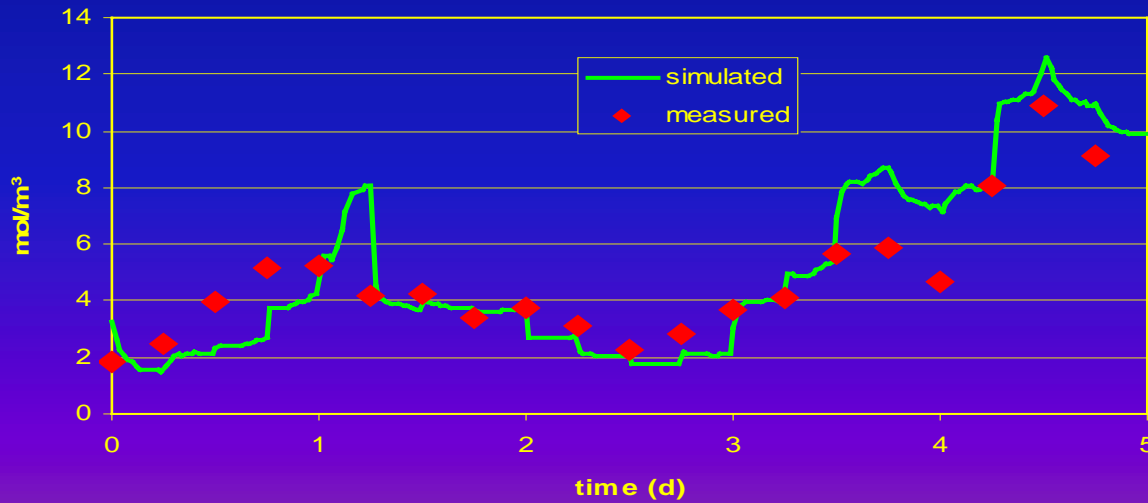
$$(K_L a)^{\text{CO}_2} \approx 0.9 * (K_L a)^{\text{O}_2}$$

1, 2 and 3 => iterative process !

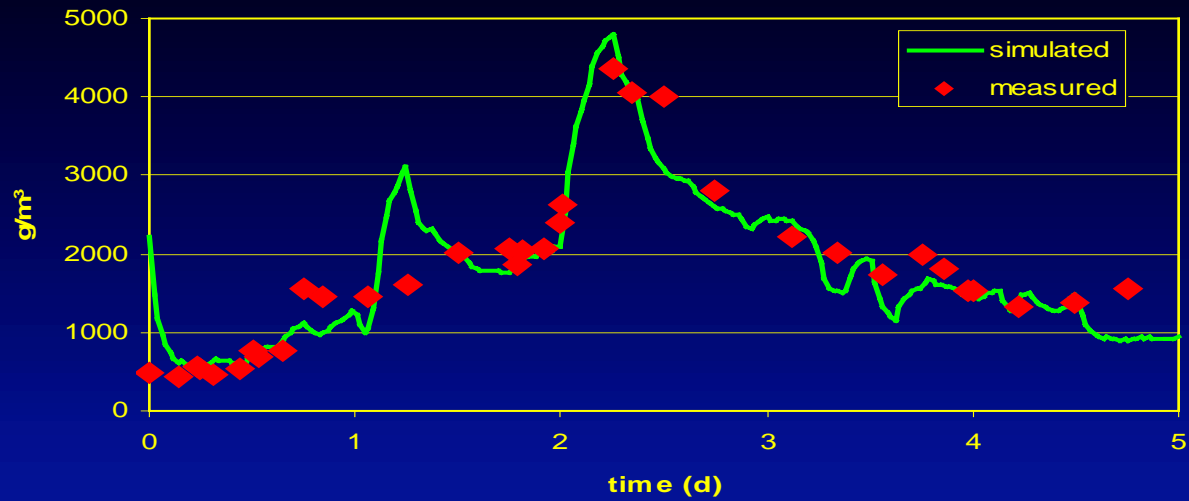
off-gas CO₂



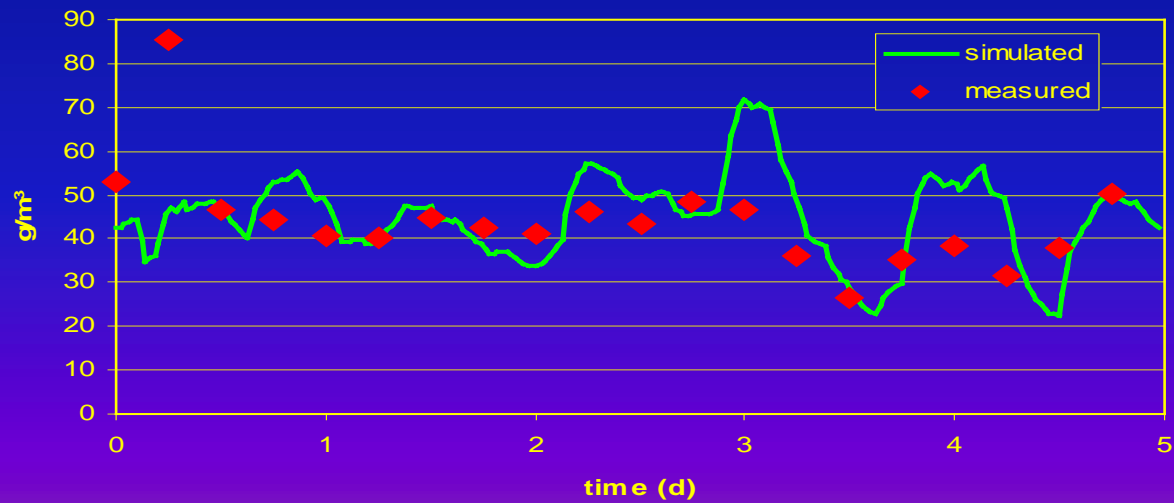
effluent HCO₃⁻



effluent readily biodegradable substrate



effluent ammonia



Conclusions

- Biofilm model building
 - A lot of models are available
 - Compromise between complexity and calibration effort is to be found
 - Model used should be dependent on the goal of the modelling study
- Model calibration
 - Iterative process, highly dependent on the available data
 - Off-line measurements sufficient for relatively simple systems
 - On-line measurements can make calibration easier
 - Respirometry: estimate biodegradable COD
 - Off-gas analysis
 - Extra information for model calibration
 - *IC* - equilibrium modelling necessary